Chemical Warfare Agent Simulants Project

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29 APRIL 2003

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Project Overview

- Background
- Purpose/Objective
- Permeation of Chemical Warfare Agents (CWA) and Simulants
  - Goal/Approach
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- Potential Benefits
- Accomplishments and Status
- Summary/Conclusion

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Project Purpose / Objective

- Purpose of Simulant Permeation Study:

  Through research and testing, identify chemical compounds to simulate the penetration and permeation effects of CWA (GB and HD) through barrier materials.

- Objective:

  Identify simulants and laboratory procedures that can be used by manufacturers for estimating CWA permeation through barrier materials used to manufacture respirators.

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Goal: Low cost, rapid, simulant screening method for determining agent barrier performance.

Approach:

1) Develop an inexpensive permeation system with a new cell design for testing both hard and soft materials up to at least 1 cm thick.

2) Select relatively nontoxic simulants for HD and GB based on solubility in standard polymers.

3) Employ permeation of agents and selected simulants to develop criteria for predicting resistance to agent penetration.

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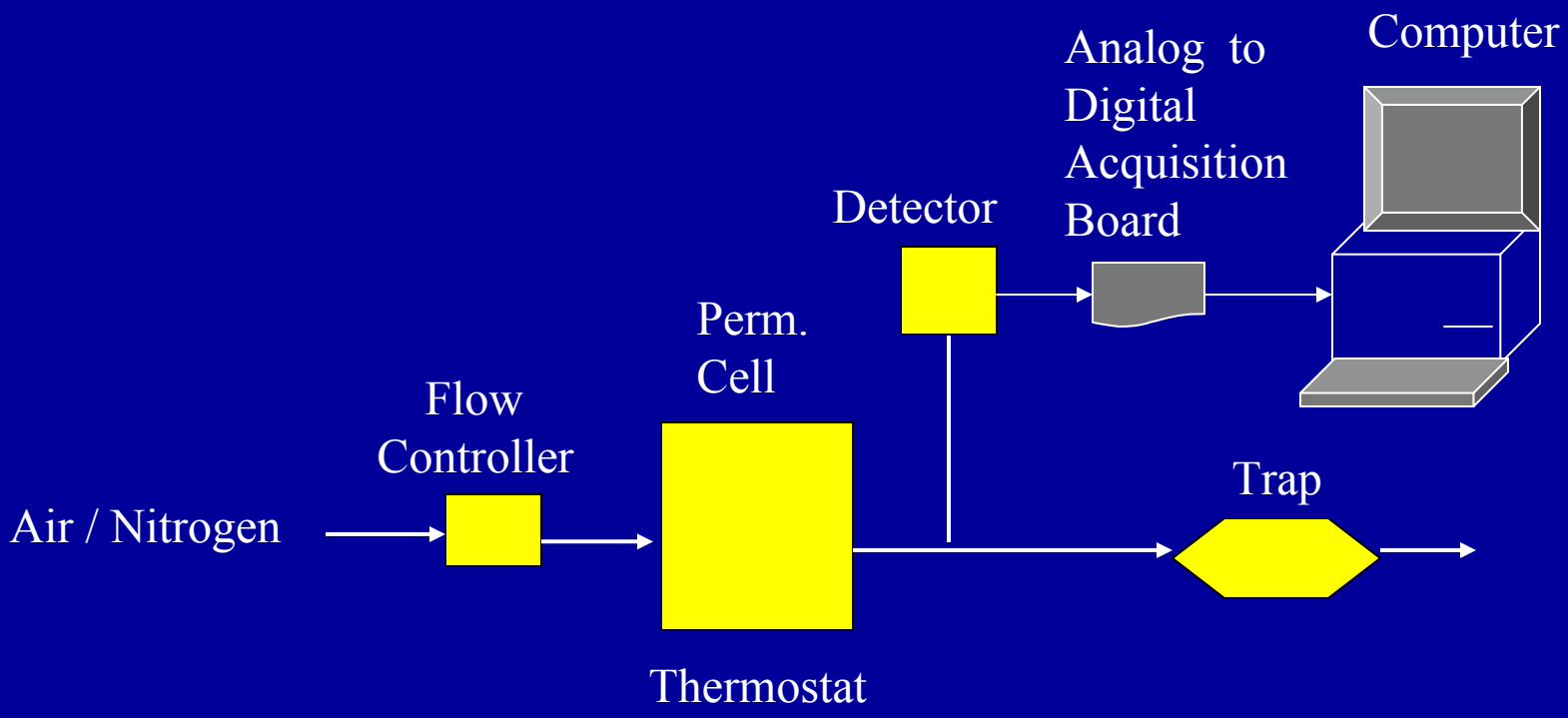
Technical Details

Permeation Test System



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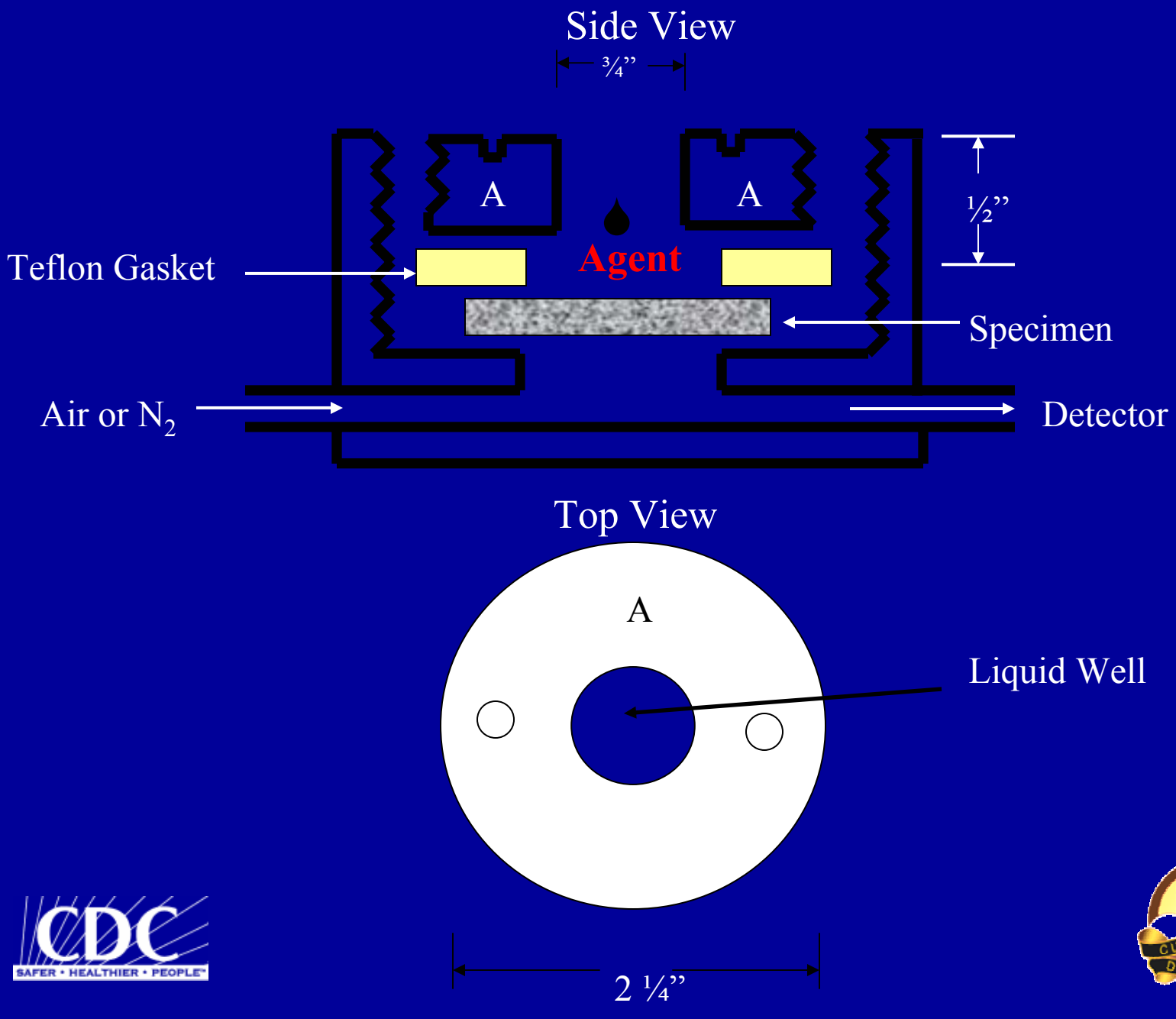
Liquid Permeation Cell



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Permeation Cell Photographs

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The Selection of Elastomeric Barrier Materials

Permeation and immersion testing was conducted on seven reinforced, cured elastomer compounds known to span a wide range in barrier properties. Three were chosen as standard materials for comparative testing with CWA (HD, GB) and simulants. The test materials with specimen thickness selected for convenient breakthrough time are:

Butyl Rubber: 12 mil
EPDM: 30 mil
Silicone Rubber: 125 mil

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Permeability (P) of Organic Molecules in Polymers via Solution - Diffusion

$$P = D \bullet S \bullet L^{-1}$$

For each polymer at a specified temperature:

Diffusion Coefficient (D) = f(molecular size, concentration)

Equilibrium Solubility (S) = f(chemical interaction, concentration)

Specimen Thickness = L

Simulants which are of comparable molecular size and have a solubility similar to that of agents in the materials of interest will provide the most reliable prediction of agent permeation.

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Liquid Simulant Candidates

HD Simulants

DCH* - 1,6-Dichlorohexane

DBSS – Di-n-butyl disulfide

BCBE – Bis 4-chlorobutyl ether

CEPS* - 2-Chloroethyl phenyl sulfide

CECS - 2-Chloroethyl cyclohexyl sulfide

DBS - Dibutyl sulfide

GB Simulants

DMMP – Dimethyl methylphosphonate

DEMP* – Diethyl methylphosphonate

DEEP – Diethyl ethylphosphonate

DIMP* - Diisopropyl methylphosphonate

TEP – Triethyl phosphate

* selected permeants

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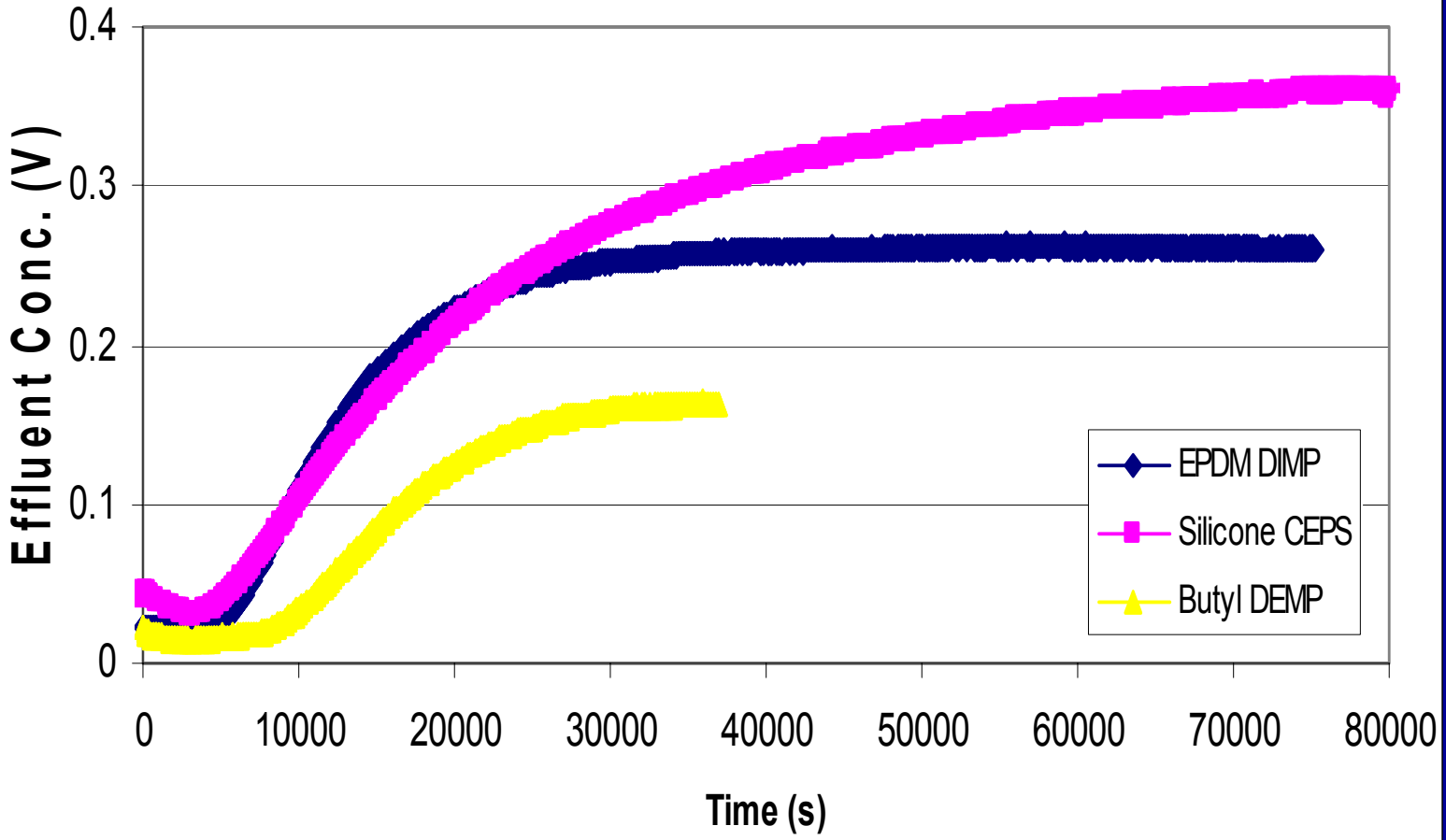
Actual Permeation Results Using the Permation Cell @ 35 C



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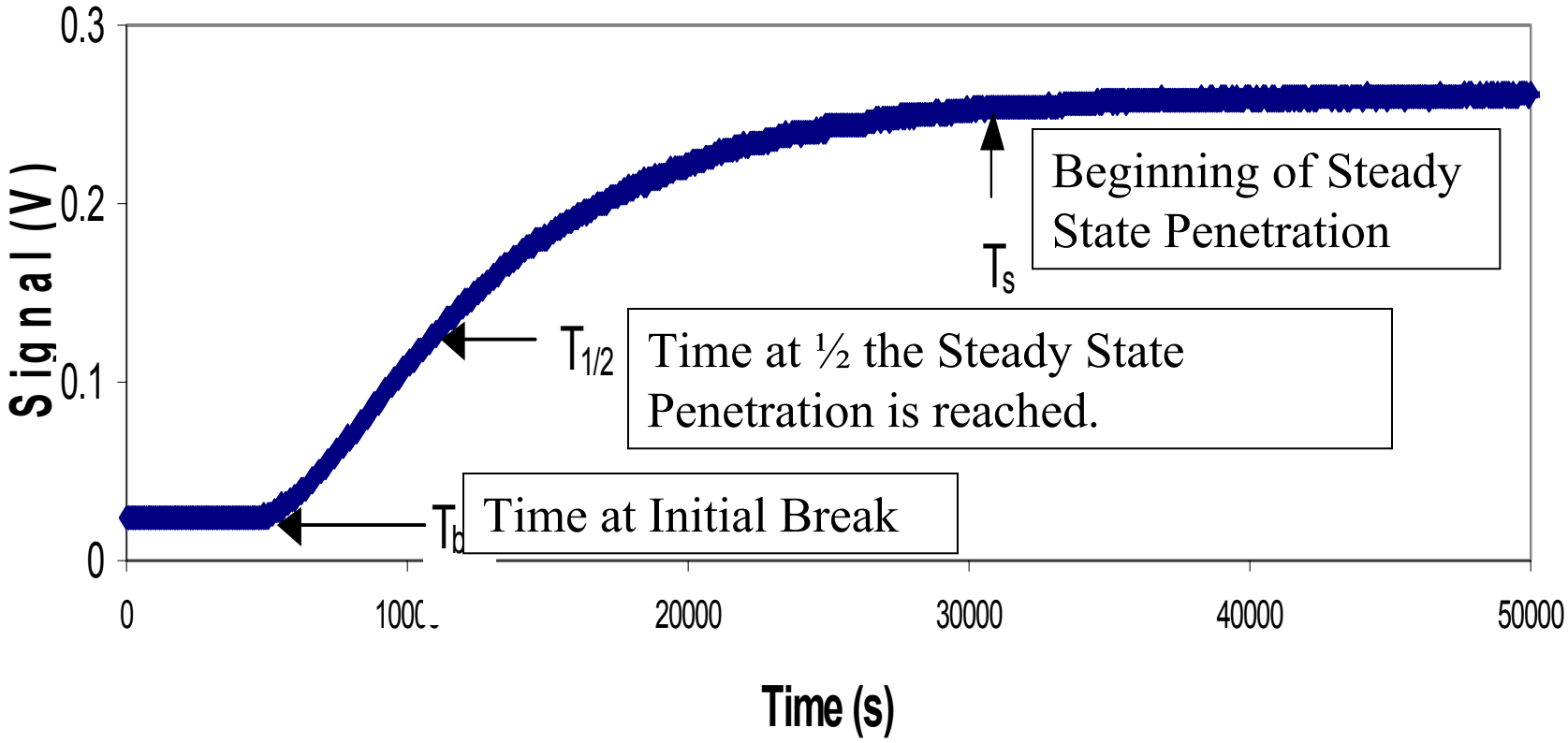
Liquid Permeation of the EPDM With DIMP



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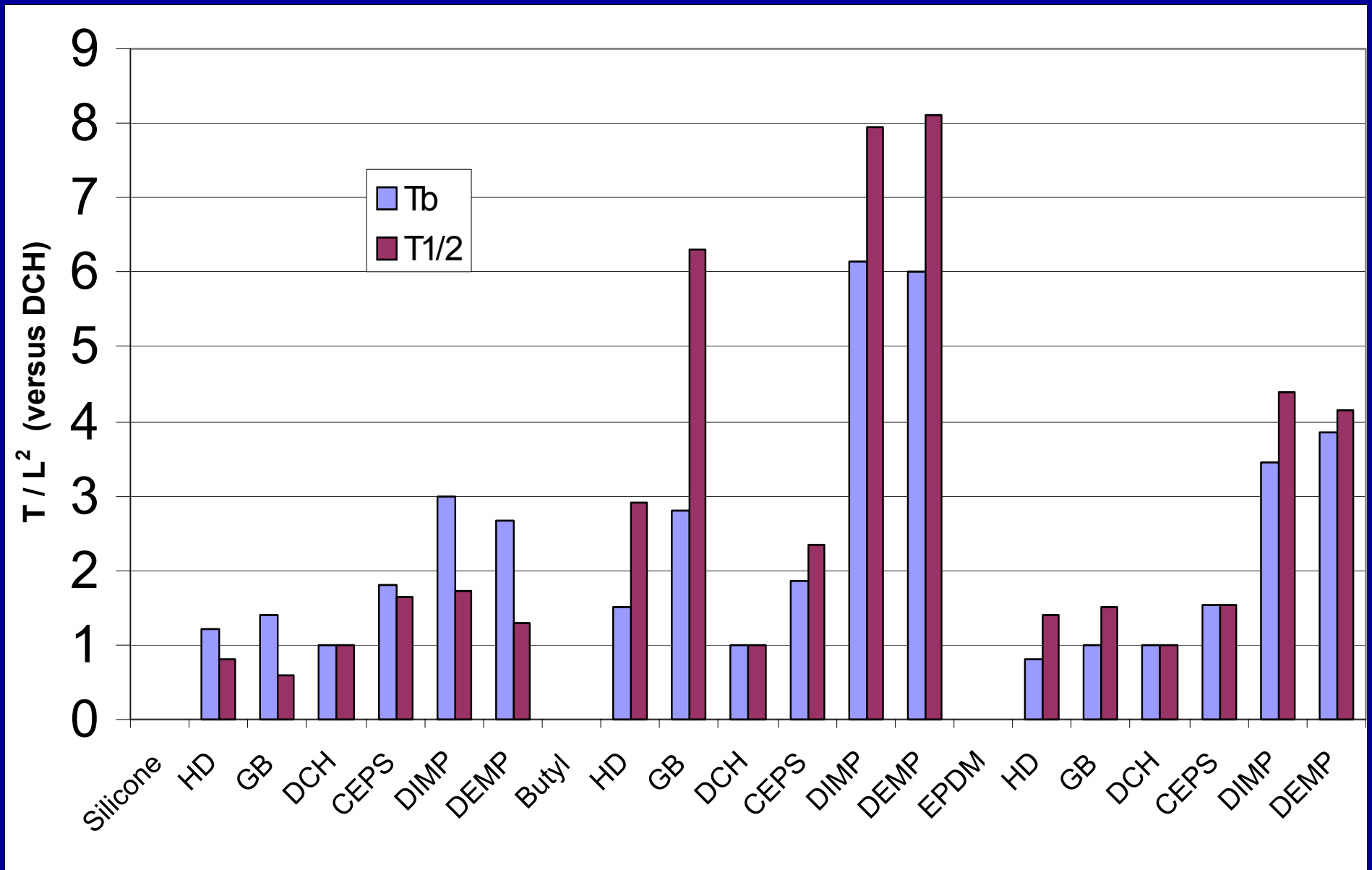
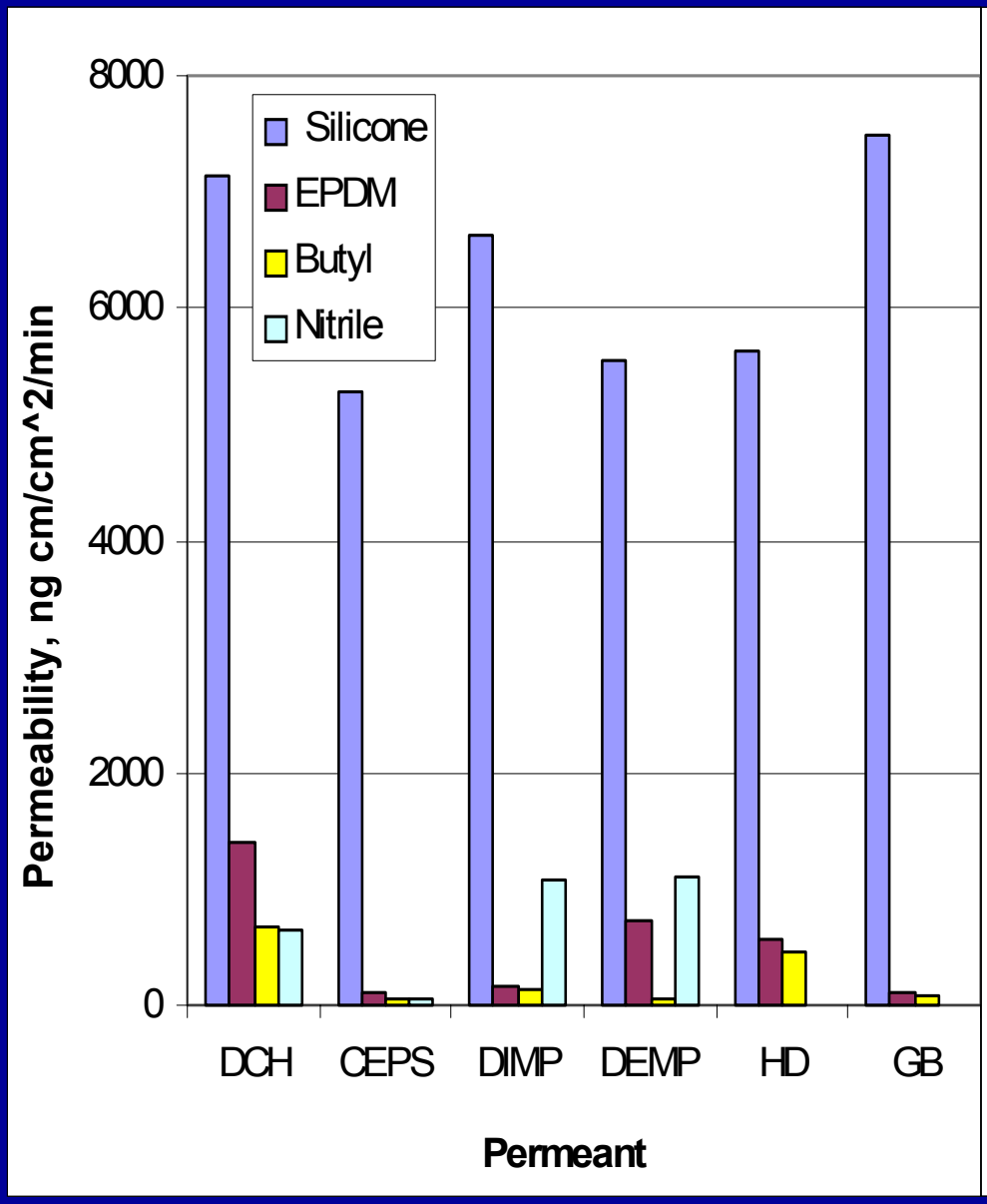
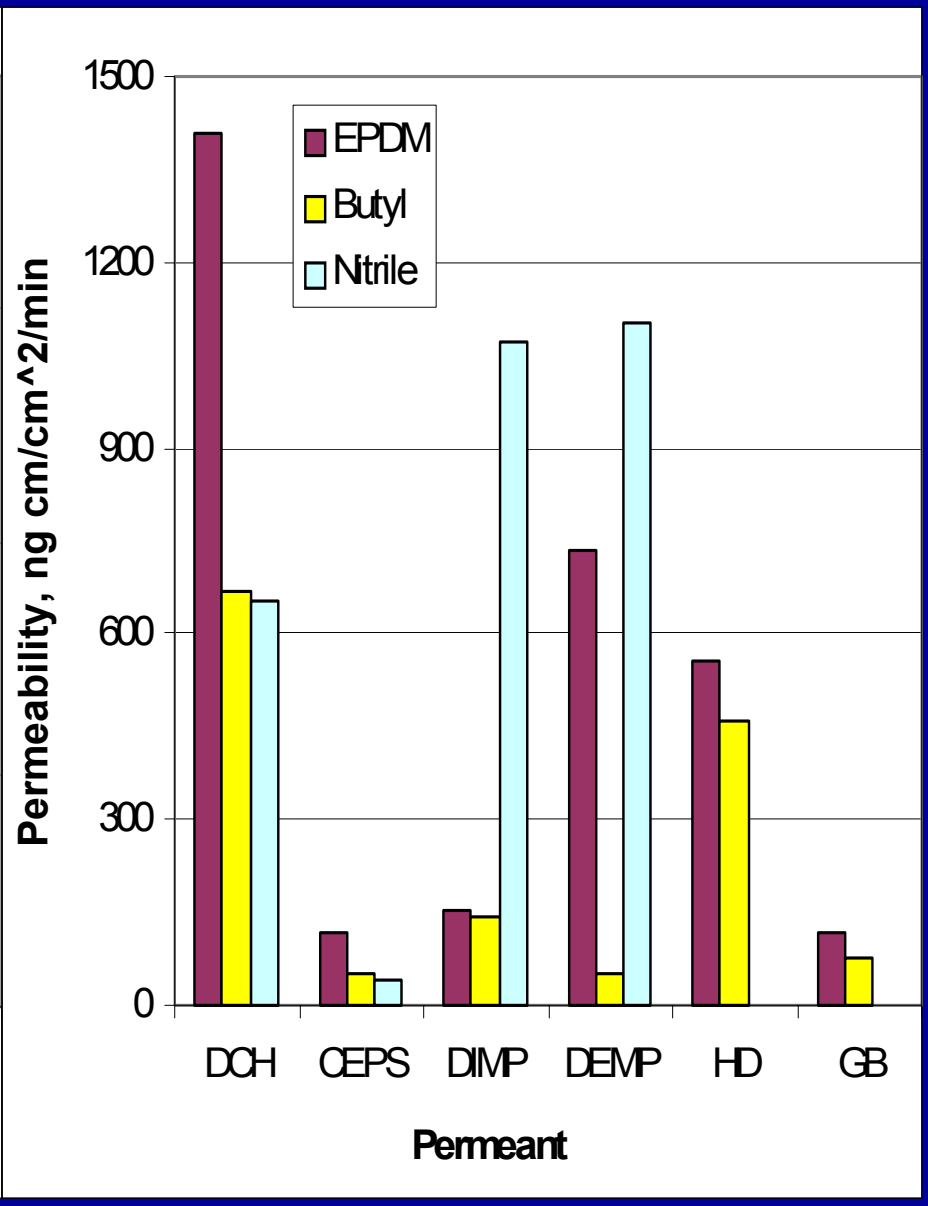
NORMALIZED CHARACTERISTIC TIME vs DCH VALUE FOR EACH ELASTOMER

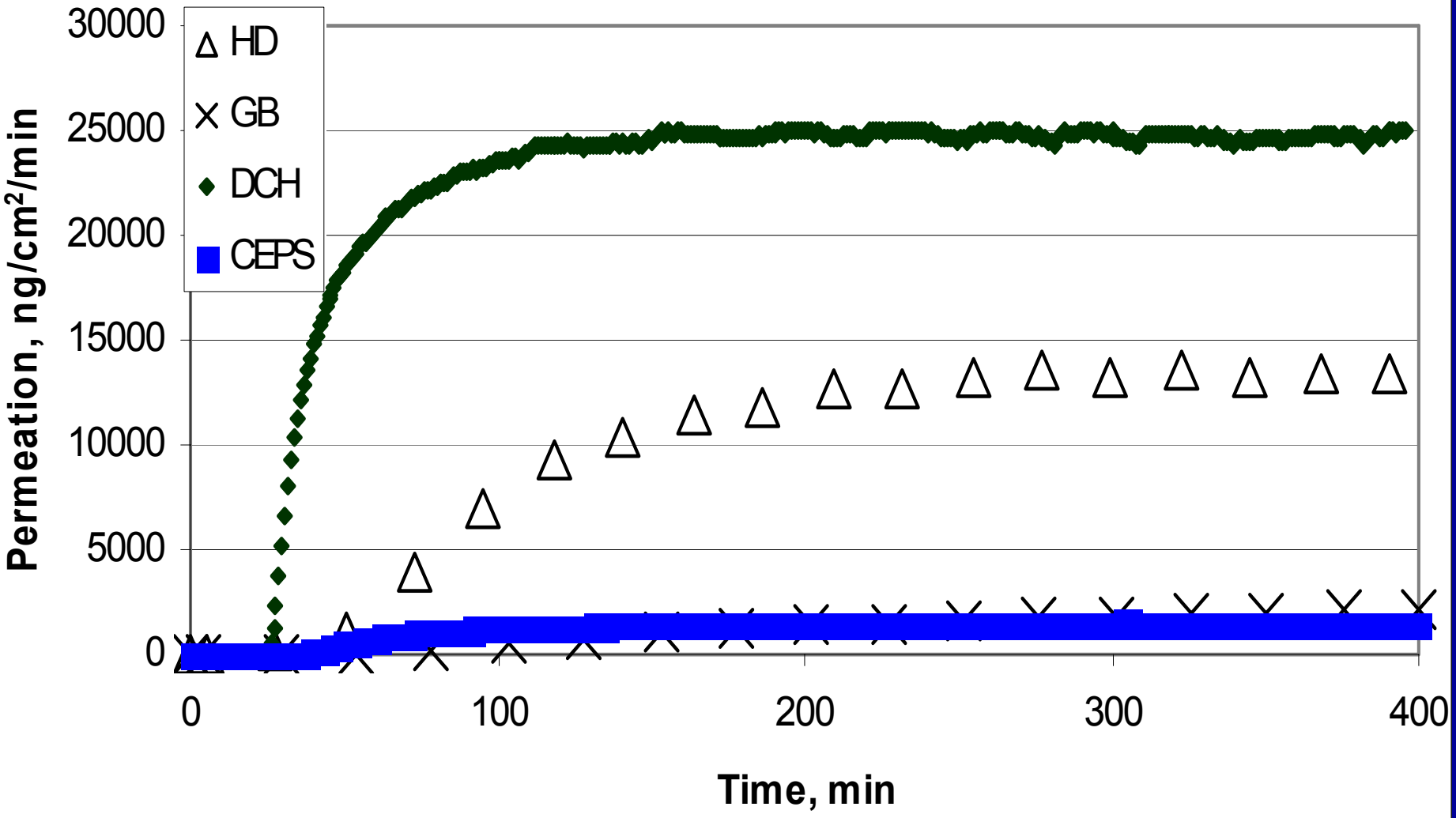


AVERAGE PERMEABILITY a) FOUR ELASTOMERS b) EXCLUDING SILICONE





PERMEATION in BUTYL RUBBER (12 mil)



Accomplishments and Current Status

Accomplishments:

1. Developed Permeation Test Method
2. Designed Convenient Permeation Cell
3. Correlated Permeation of CWA and Simulants
4. Recommended Criteria for Evaluating Barrier Properties Using Simulants
5. Wrote NIOSH Draft Working Documents: "Liquid Permeation Through Nonporous Materials" and "Test Method For Liquid Permeation Through Nonporous Polymer"

Status: Convenient Method Available for Testing with Simulants or Toxic Liquids

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Benefits of Simulant Permeation Study:

1. Provides basis for determining suitable simulants for evaluating materials of construction.

2. Assists manufacturers in selection of barrier materials based on scientific information, reducing product development time and cost.

3. Expedites availability of new respirators and materials technology for the users.

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Summary/Conclusion

- Identified simulants and a rapid, relatively low cost laboratory procedure that can be used by manufacturers for estimating CWA permeation through barrier materials.

- Wrote a draft NIOSH Guidance Document that describes test procedures, and results of agent and simulant permeation tests.

- NIOSH or SBCCOM do not guarantee that simulants identified will be suitable for all materials, nor does passage of manufacturer's pretest with a simulant guarantee passage of the official NIOSH certification testing.

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